MS82
Scalable Dynamical Cores for Climate and Weather Modeling

Title not available at time of publication

Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U. S. Department of Energy under Contract No. DE-AC05-00OR22725.

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Overcoming the Time Barrier

Rick Archibald, John Drake, Kate Evans, Doug Kothe, Trey White, Pat Worley

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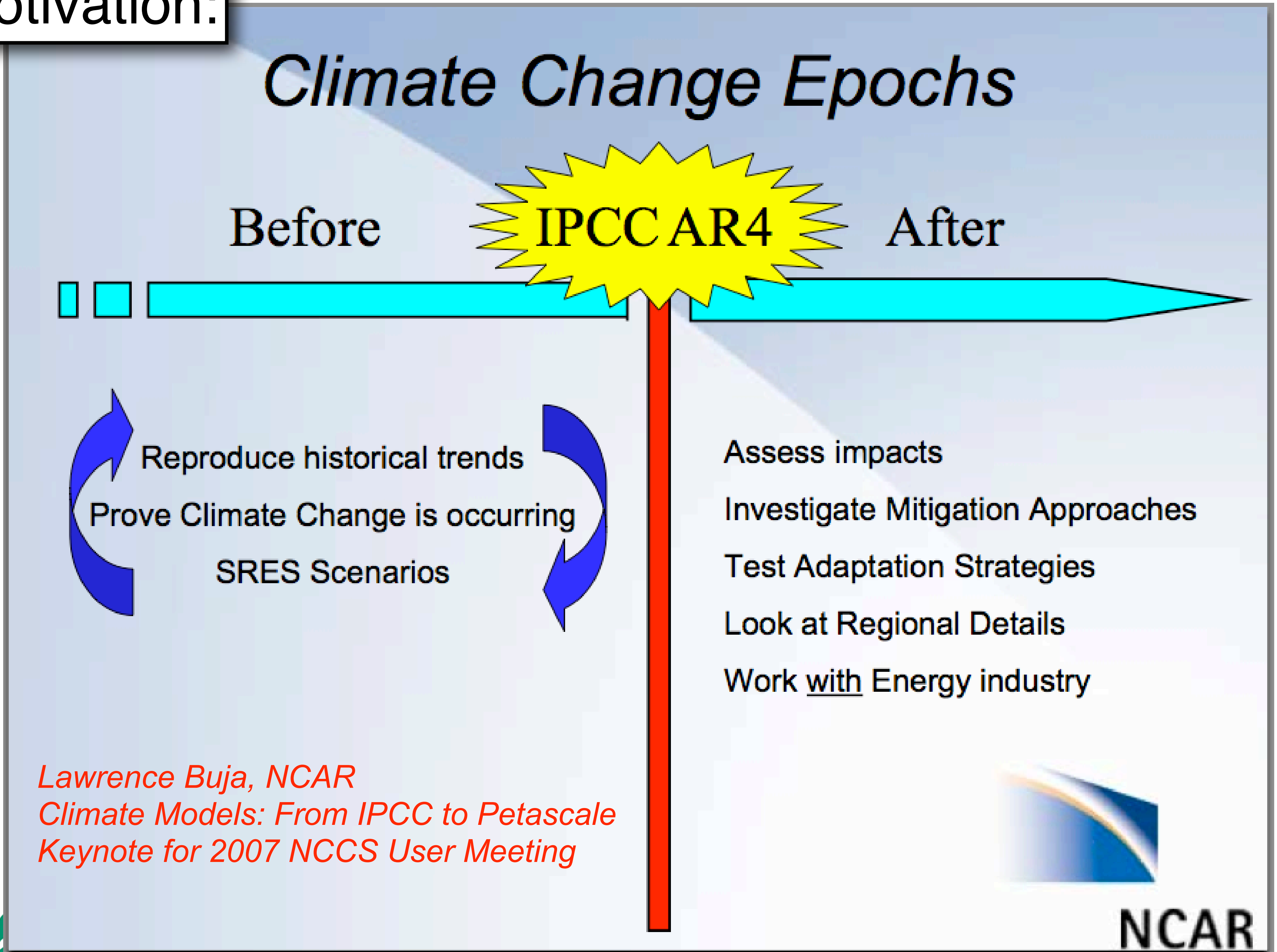
Oak Ridge National Laboratory

Motivation:



Climate Change Epochs
Before
IPCC AR4
After
Reproduce historical trends
Prove Climate Change is occurring
SRES Scenarios
Assess impacts
Investigate Mitigation Approaches
Test Adaptation Strategies
Look at Regional Details
Work with Energy industry
Lawrence Buja, NCAR
Climate Models: From IPCC to Petascale
Keynote for 2007 NCCS User Meeting
NCAR

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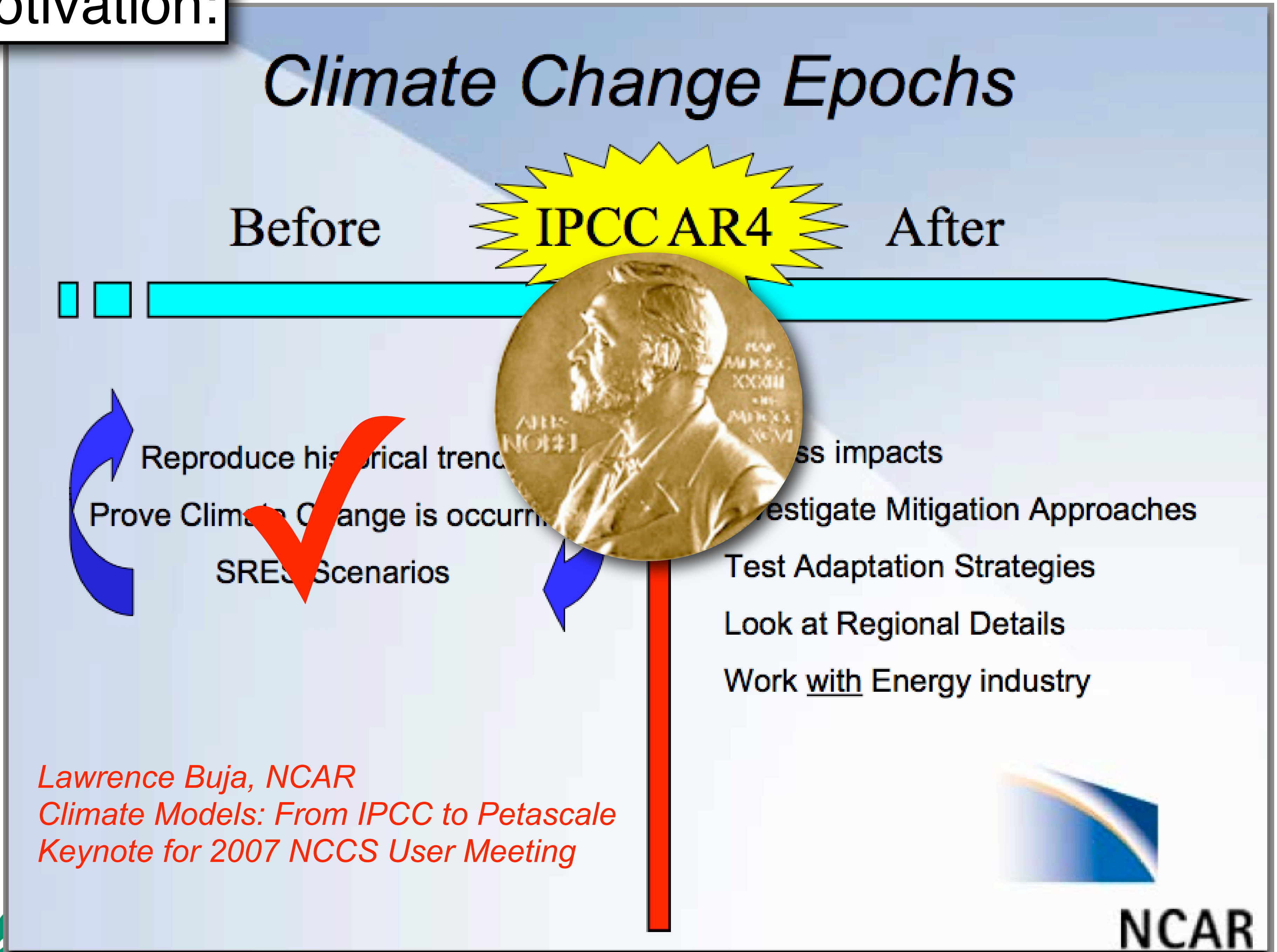

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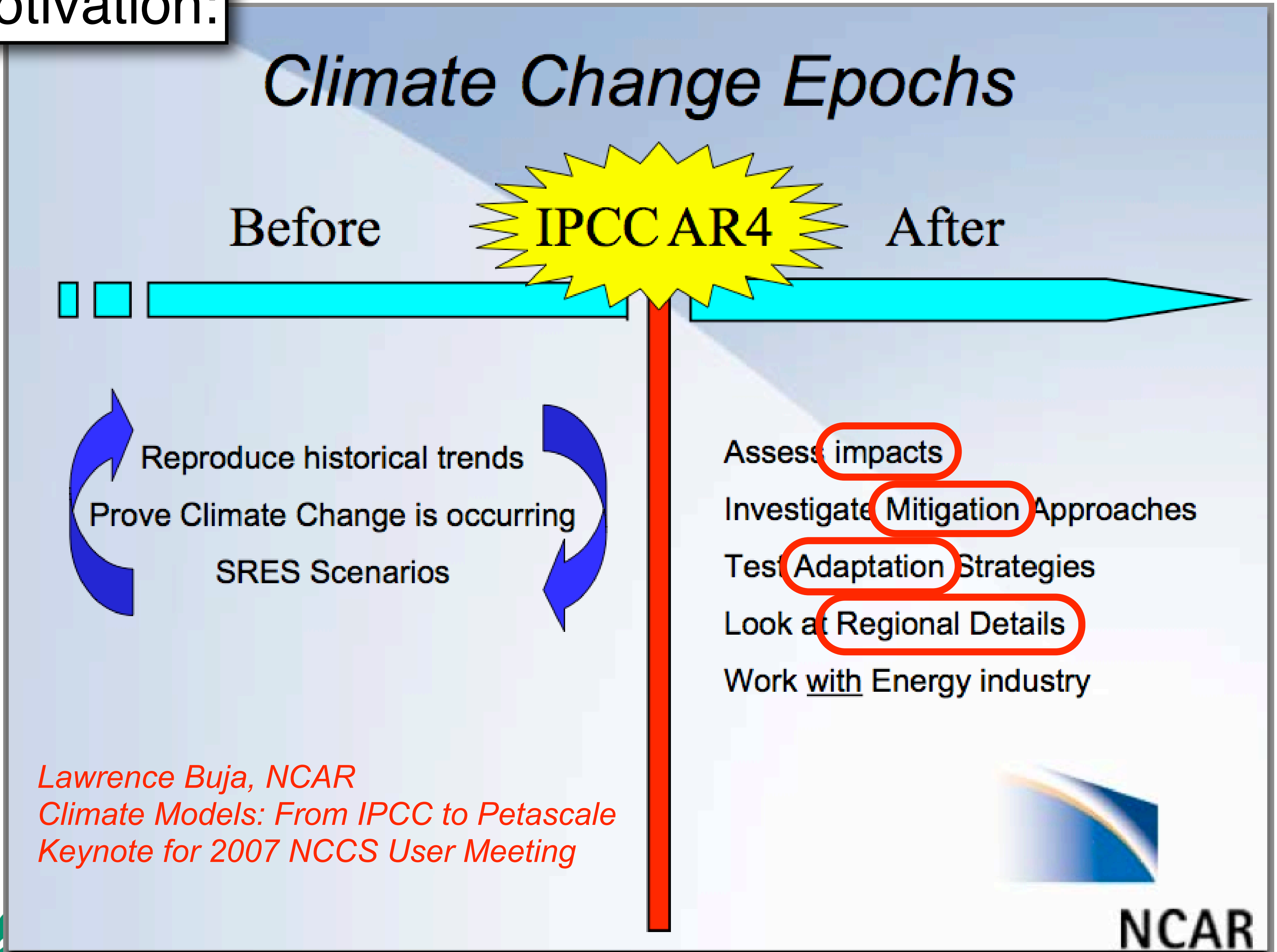
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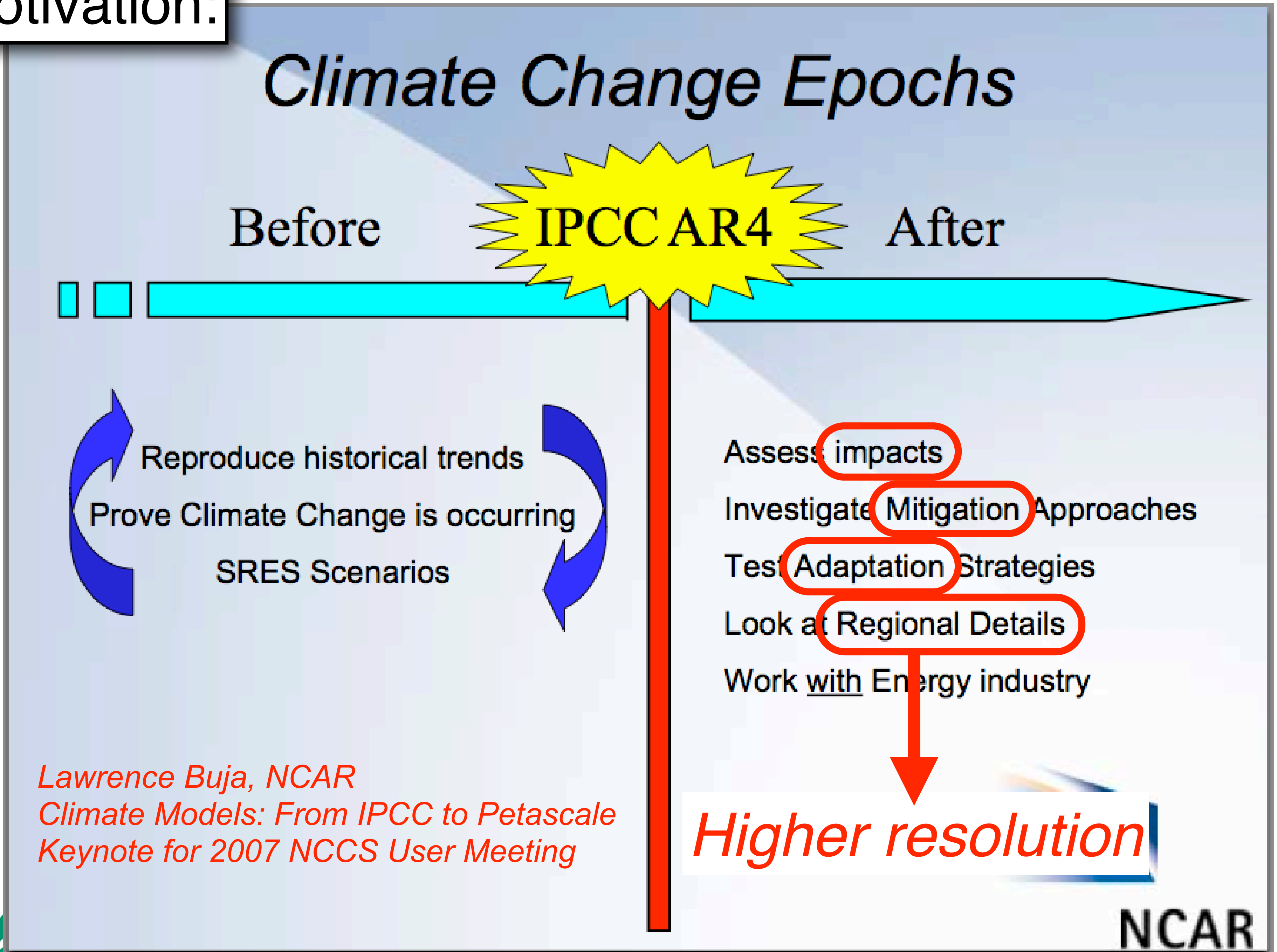

Climate Change Epochs
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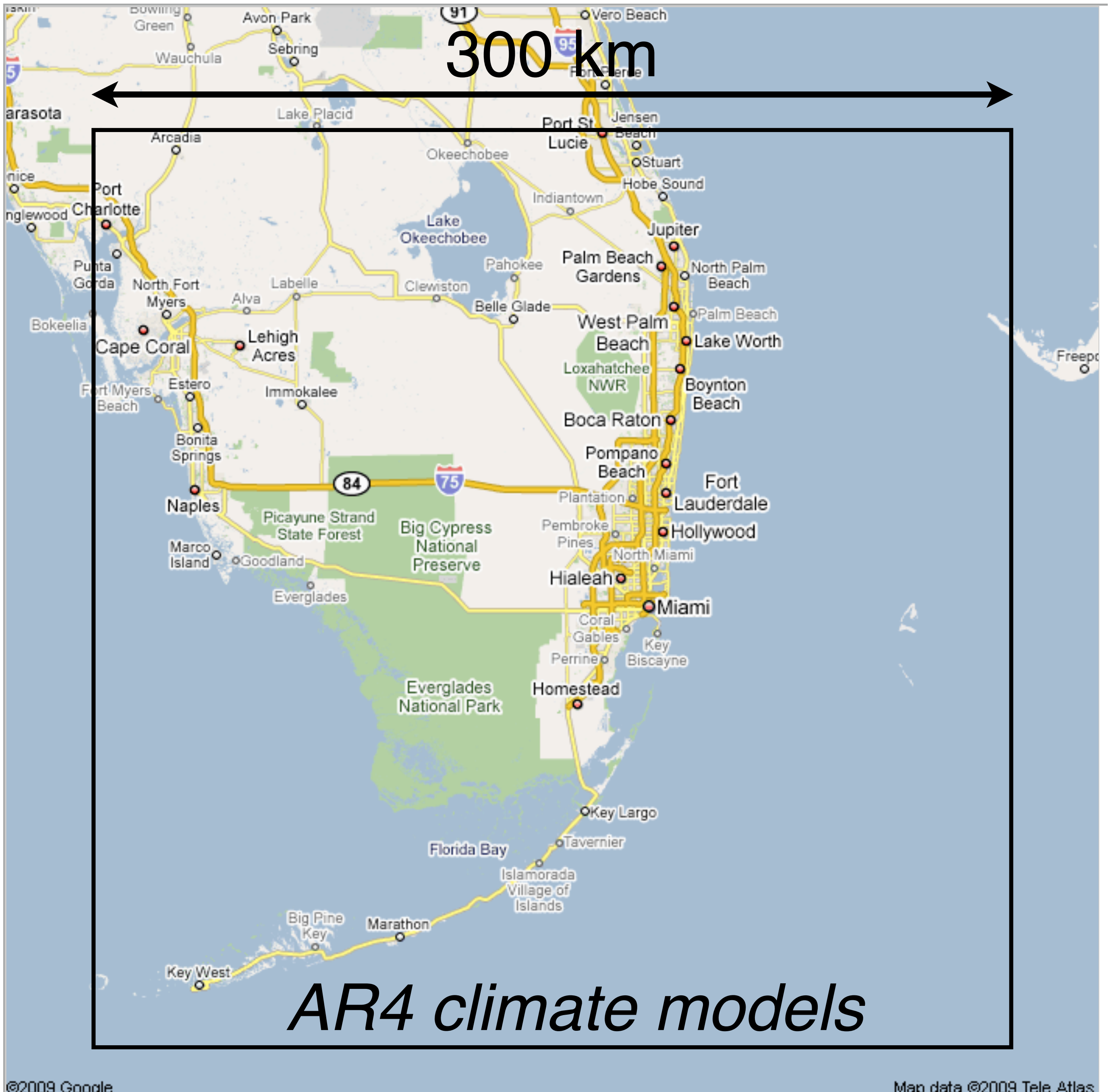
Higher resolution
NCAR


300 km
AR4 climate models
Vero Beach
Avon Park
Sebring
Wauchula
Lake Placid
Arcadia
Okeechobee
Port St. Lucie
Jensen Beach
Stuart
Hobe Sound
Port Charlotte
Indiantown
Lake Okeechobee
Jupiter
Punta Gorda
North Fort Myers
Labelle
Pahokee
Palm Beach Gardens
North Palm Beach
Clewiston
Alva
Belle Glade
Palm Beach
Bokeelia
Cape Coral
Lehigh Acres
West Palm Beach
Lake Worth
Loxahatchee NWR
Estero
Immokalee
Boynton Beach
Fort Myers Beach
Boca Raton
Bonita Springs
Pompano Beach
84
75
Fort Lauderdale
Naples
Plantation
Picayune Strand State Forest
Big Cypress National Preserve
Pembroke Pines
Hollywood
Marco Island
Goodland
North Miami
Everglades
Hialeah
Miami
Coral Gables
Key Biscayne
Perrine
Everglades National Park
Homestead
Key Largo
Florida Bay
Tavernier
Islamorada Village of Islands
Big Pine Key
Marathon
Key West
Freeport
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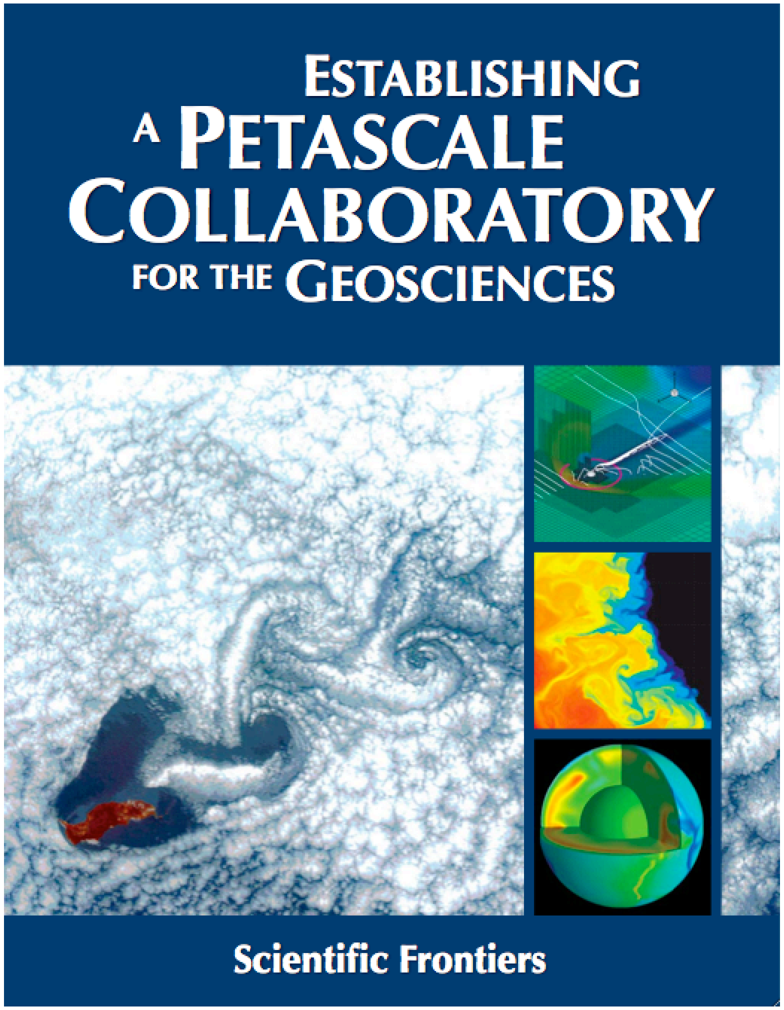
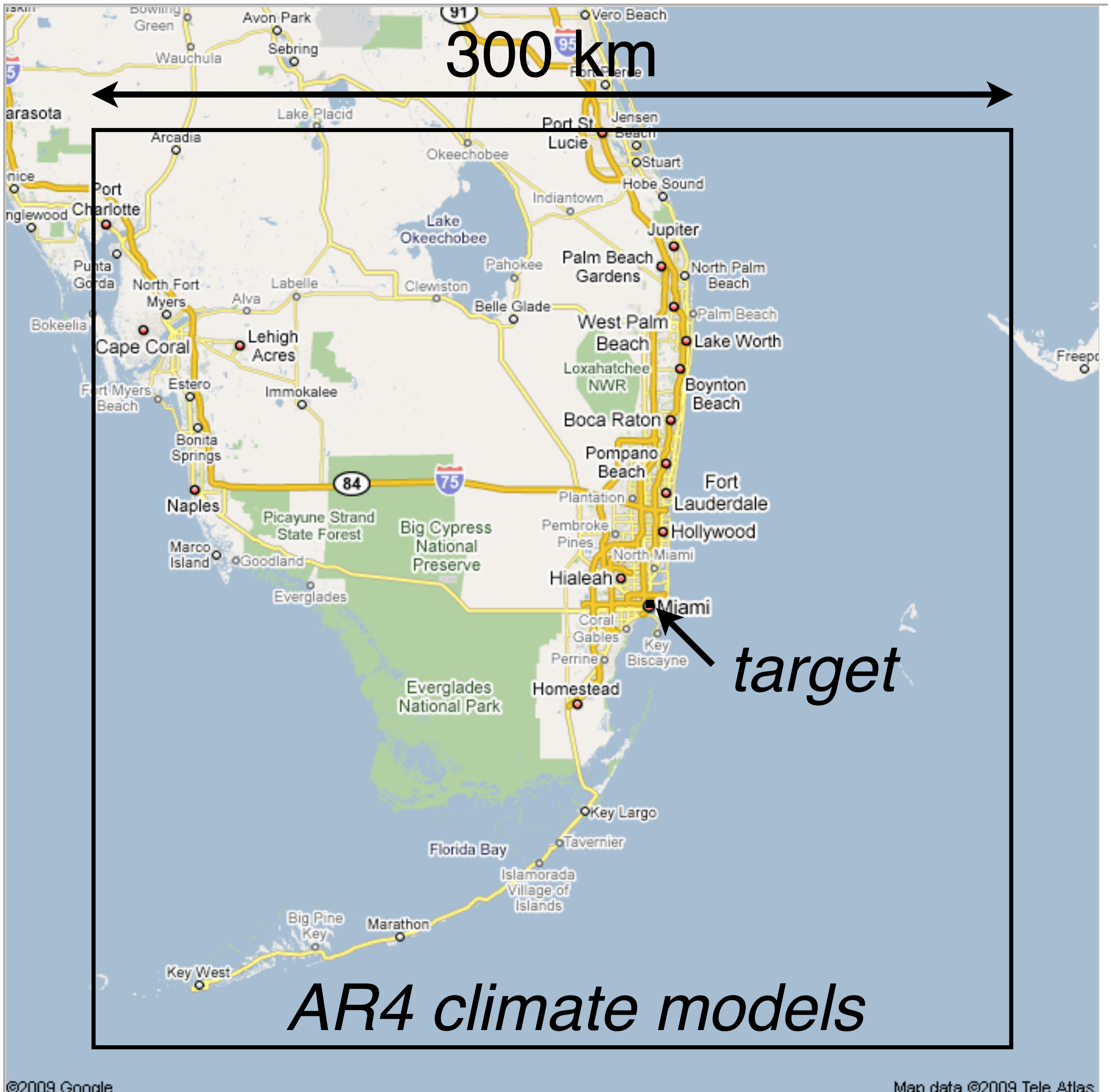


"More importantly, because the assumptions that are made in the development of parameterizations of convective clouds and the planetary boundary layer are seldom satisfied, the atmospheric component model must have sufficient resolution to dispense with these parameterizations. This would require a horizontal resolution of 1 km."

http://www.geo-prose.com/projects/pdfs/petascale_science.pdf


300 km
target
AR4 climate models
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Sebring
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Big Pine Key
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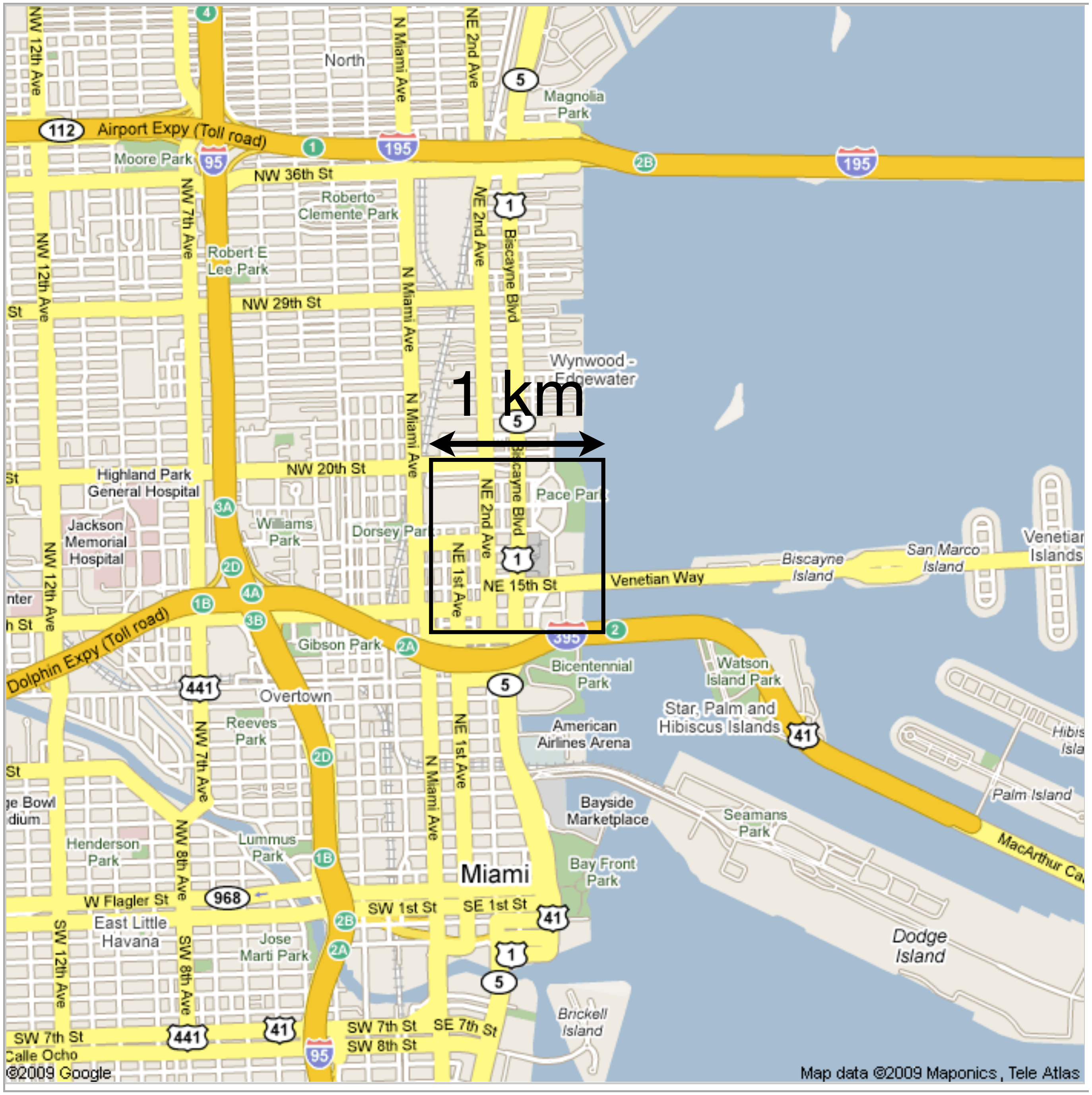
1 km
North
Airport Expy (Toll road)
Moore Park
NW 36th St
Roberto Clemente Park
Robert E Lee Park
NW 29th St
Magnolia Park
Wynwood - Edgewater
NW 20th St
Highland Park General Hospital
Jackson Memorial Hospital
Williams Park
Dorsey Park
Pace Park
NE 15th St
Venetian Way
Biscayne Island
San Marco Island
Venetian Islands
Dolphin Expy (Toll road)
Gibson Park
Overtown
Reeves Park
Bicentennial Park
Watson Island Park
Star, Palm and Hibiscus Islands
American Airlines Arena
Bayside Marketplace
Seamans Park
Palm Island
MacArthur Ca
Henderson Park
Lummus Park
Miami
Bay Front Park
W Flagler St
SW 1st St
SE 1st St
East Little Havana
Jose Marti Park
Dodge Island
Brickell Island
SW 7th St
SE 7th St
SW 8th St
Calle Ocho
NW 12th Ave
NW 7th Ave
NW 8th Ave
SW 12th Ave
SW 8th Ave
N Miami Ave
NE 2nd Ave
NE 1st Ave
Biscayne Blvd
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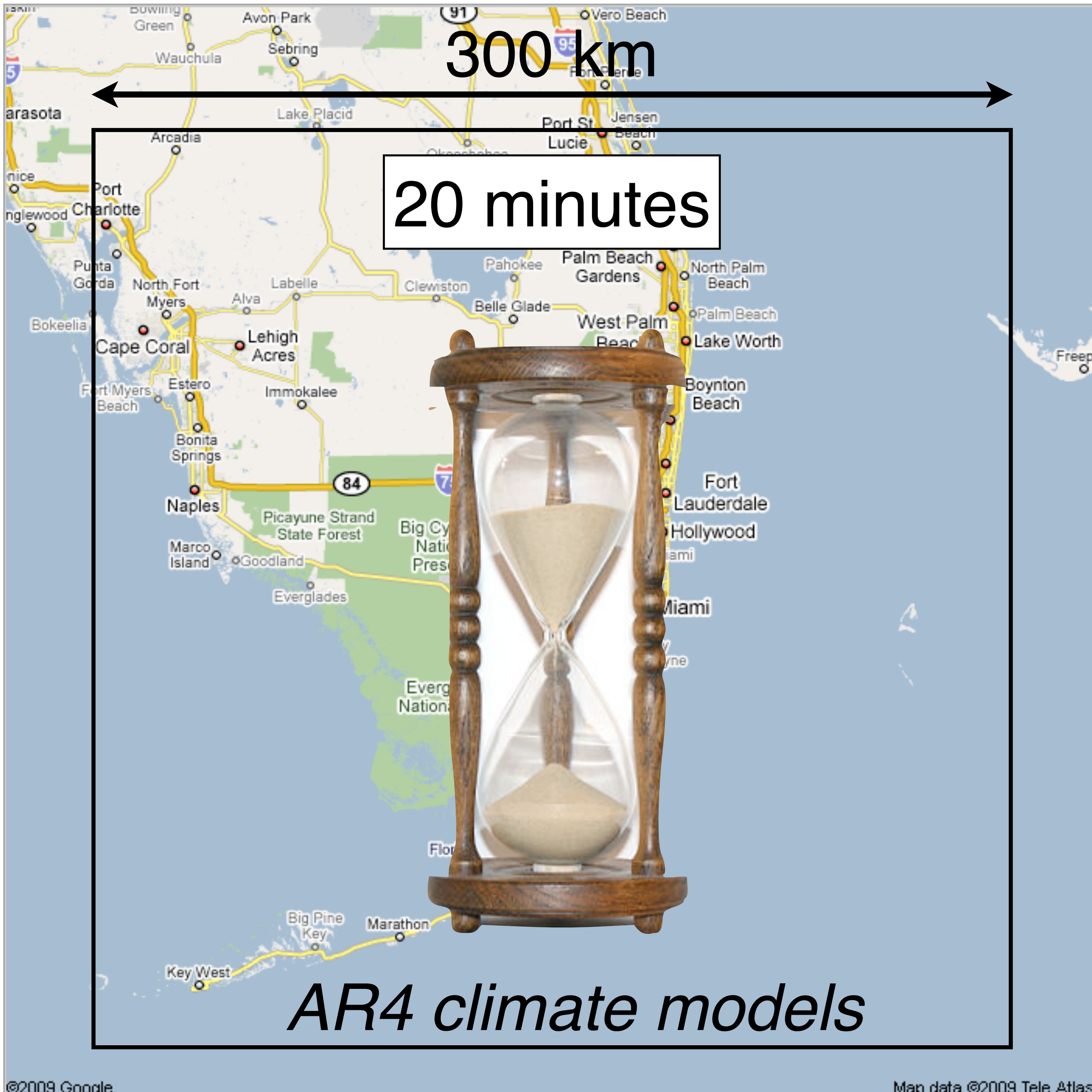
TIME BARRIER

Current climate models use ***explicit*** time integration

If resolution goes up

the time step **must** go down!


300 km
20 minutes
AR4 climate models
Avon Park
Sebring
Wauchula
Vero Beach
Lake Placid
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Port Charlotte
Punta Gorda
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Marco Island
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Everglades
Fort Lauderdale
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Key West
Freeport
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1 km
4 seconds!
EXTECH
10 LAP MEMORY
North
Magnolia Park
Airport Expy (Toll road)
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Brickell Island
SW 7th St
SE 7th St
SW 8th St
Calle Ocho
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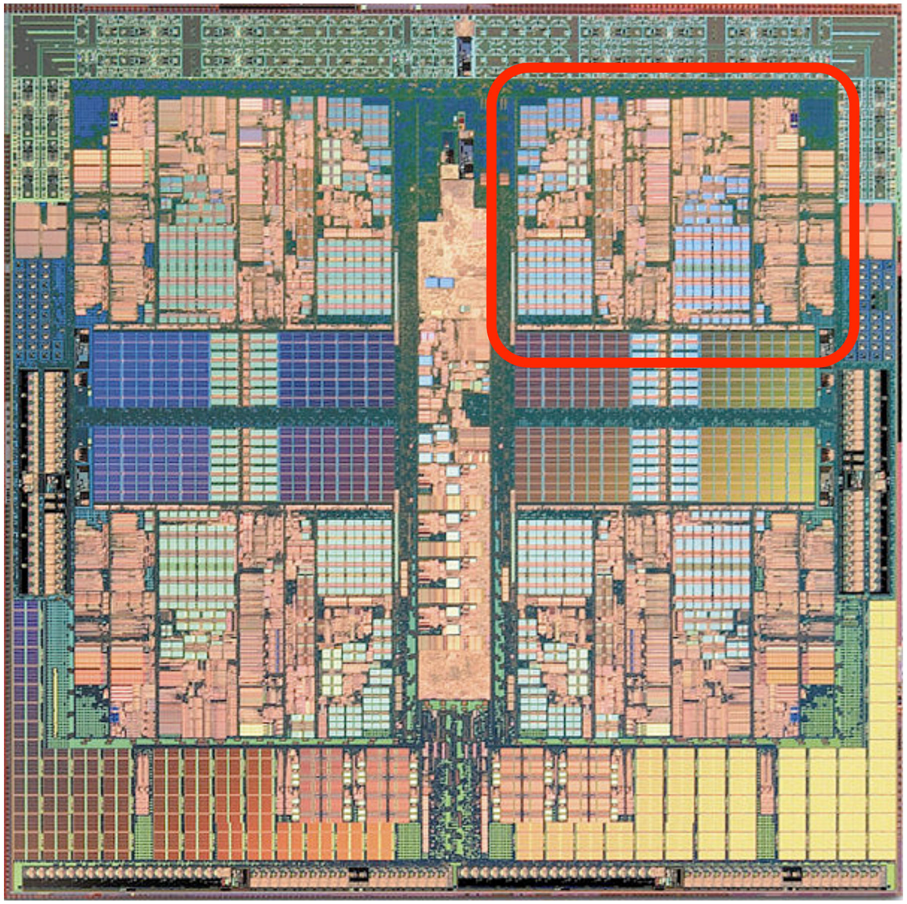
Extreme-scale systems will provide unprecedented parallelism!

But

performance of individual processes has stagnated

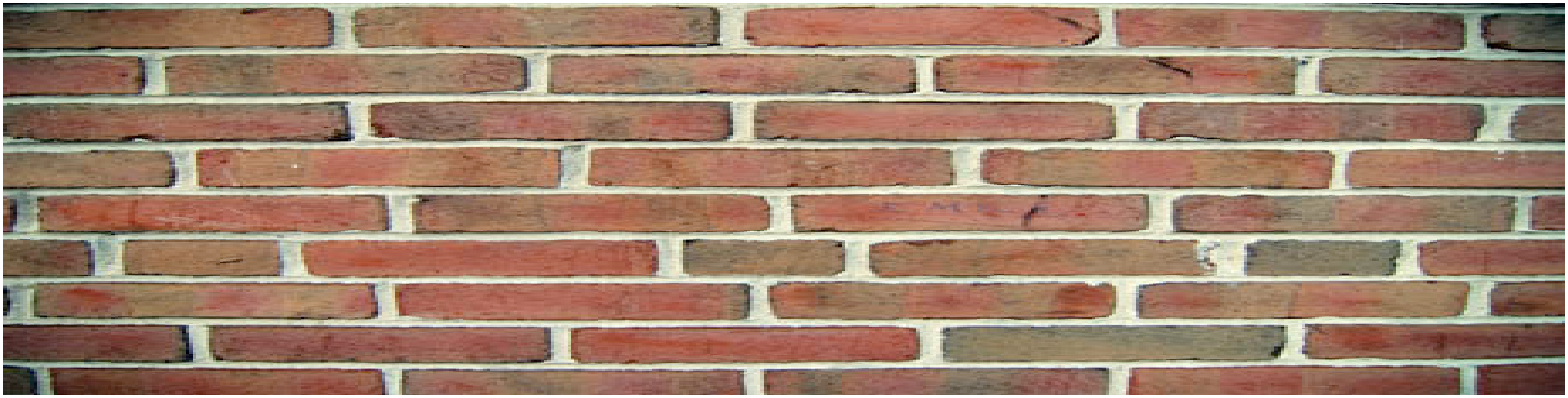


4-second
time step...

multi-century simulation?

Overcoming the time barrier

- Fully implicit time integration
- Multiwavelet discontinuous Galerkin
- Parareal



How to build a new climate model

1. Start with shallow-water equations on the sphere

$$\frac{\partial h^* \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v} h^* \mathbf{v}) = -f \hat{\mathbf{k}} \times h^* \mathbf{v} - g h^* \nabla h$$

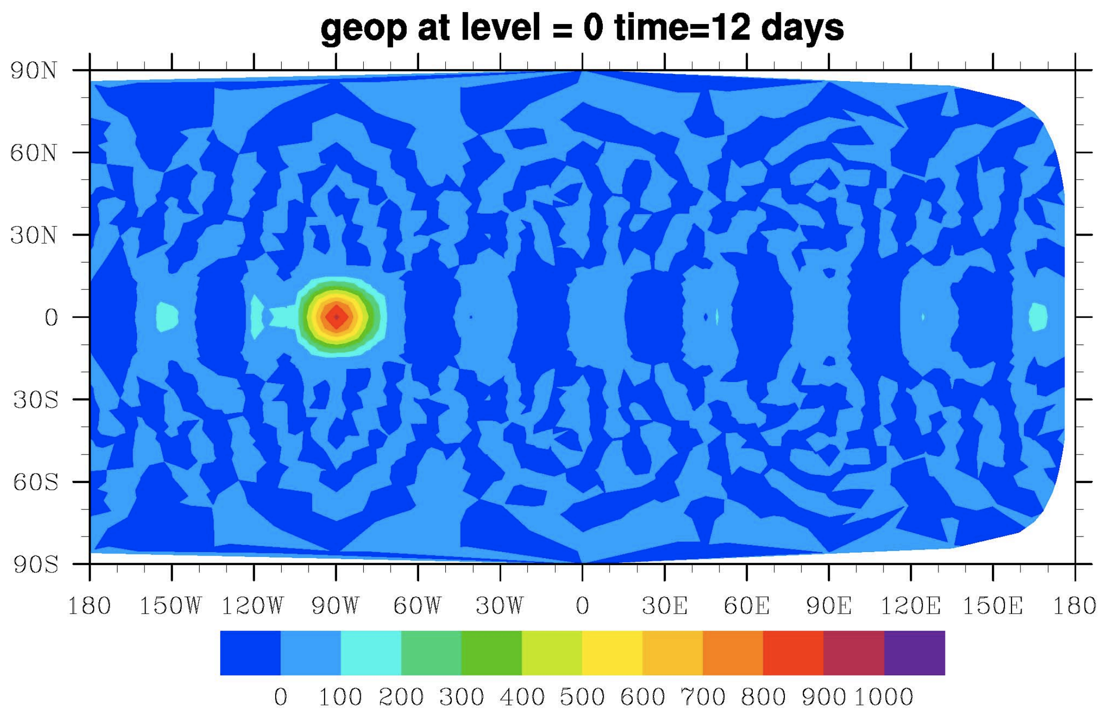
$$\frac{\partial h^*}{\partial t} + \nabla \cdot (h^* \mathbf{v}) = 0$$

$$h = h^* + h_s$$

They mimic full equations for atmosphere and ocean

How to build a new climate model

2. Prove yourself on standard tests



Defined by Williamson, Drake, Hack, Jakob, and Swarztrauber in 1992 (~150 citations)

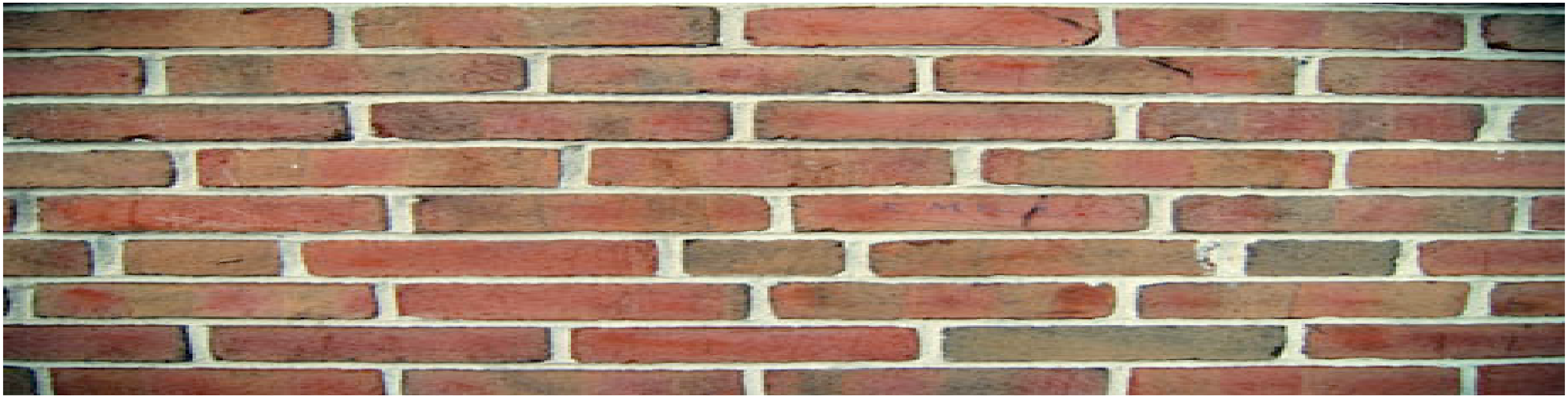
How to build a new climate model

3. Proceed to 3D tests and inclusion in a full model

That's all there is to it!

Overcoming the time barrier

- Fully implicit time integration
- Multiwavelet discontinuous Galerkin
- Parareal



Explicit good and bad

- Good
  - Highly parallel
  - Nearest-neighbor communication
- Bad
  - Numerically unstable (blows up) for $\Delta t > O(\Delta x)$
  - Increase resolution → decrease Δx → decrease Δt

Implicit bad and good

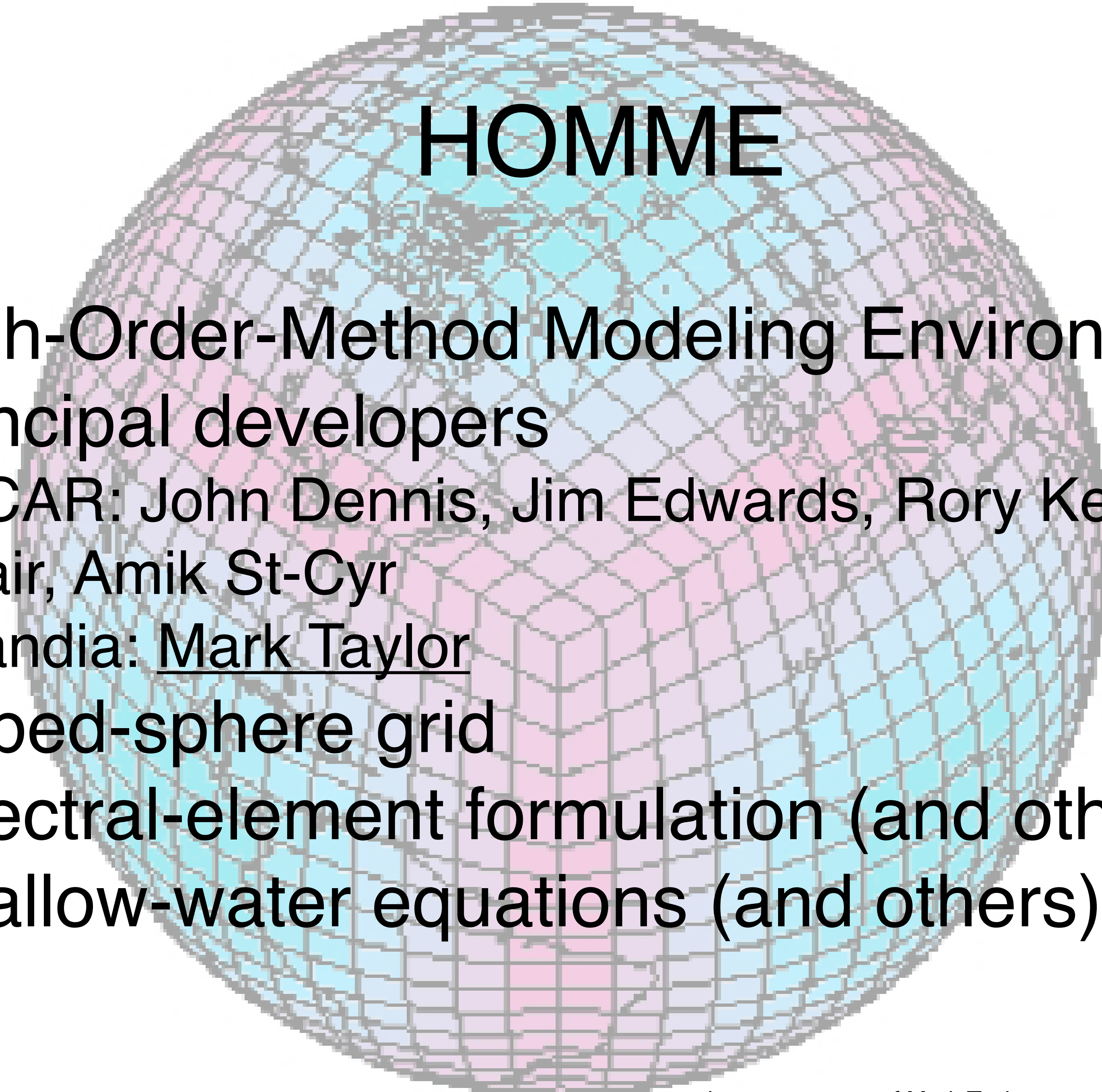
- Bad
  - Must solve a (nonlinear) system of equations
- Good
  - Numerically stable for arbitrary time steps
- Ugly
  - Still need to worry about accuracy (for big time steps)

Implicit + shallow water
(Kate Evans)

- Start with HOMME shallow-water code
- Convert explicit formulation to implicit
- Use Jacobian-Free Newton Krylov (JFNK)
- Solve with Trilinos

http://trilinos.sandia.gov/

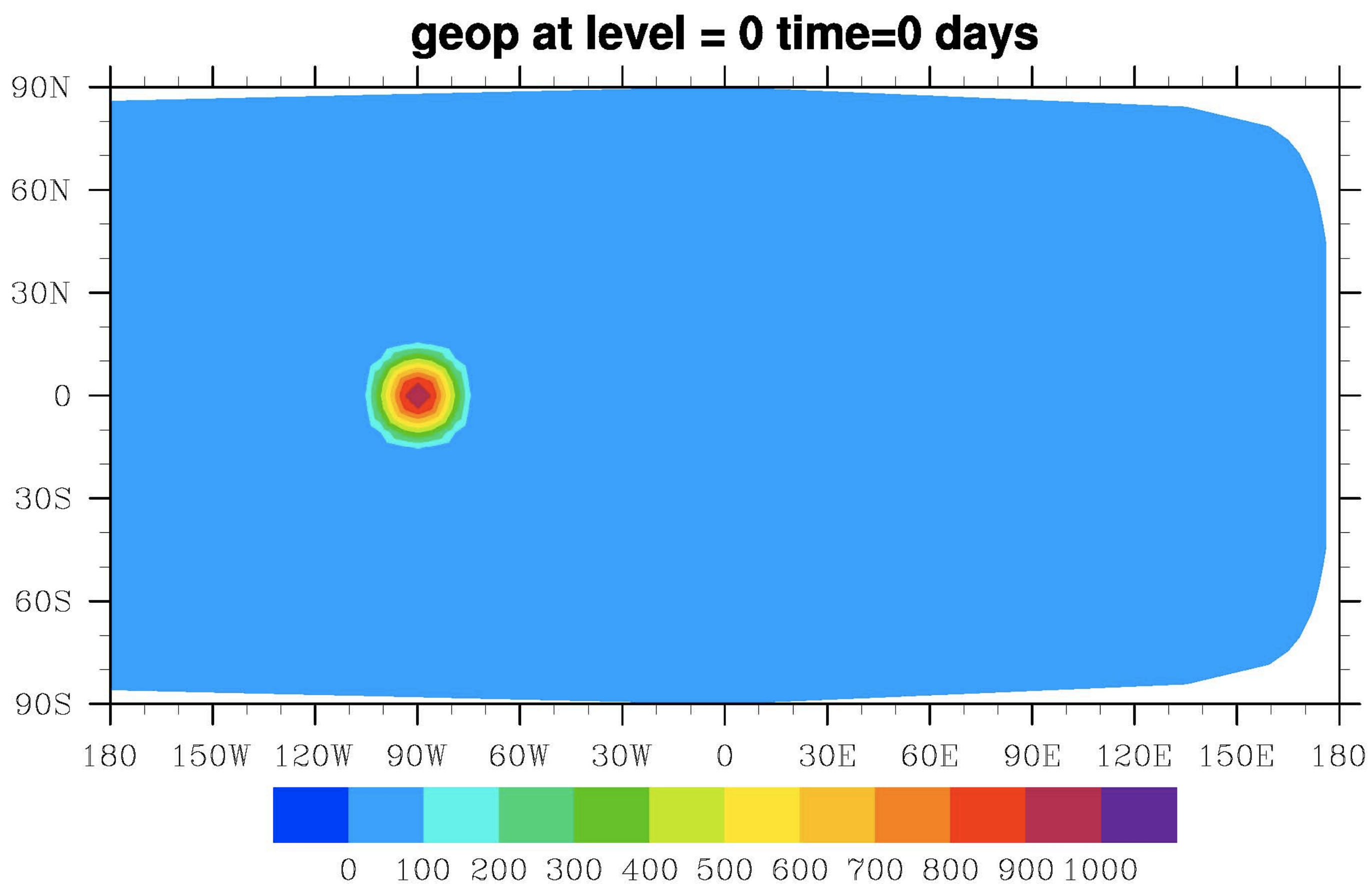
HOMME



- High-Order-Method Modeling Environment
- Principal developers
  - NCAR: John Dennis, Jim Edwards, Rory Kelly, Ram Nair, Amik St-Cyr
  - Sandia: Mark Taylor
- Cubed-sphere grid
- Spectral-element formulation (and others)
- Shallow-water equations (and others)

image courtesy of Mark Taylor

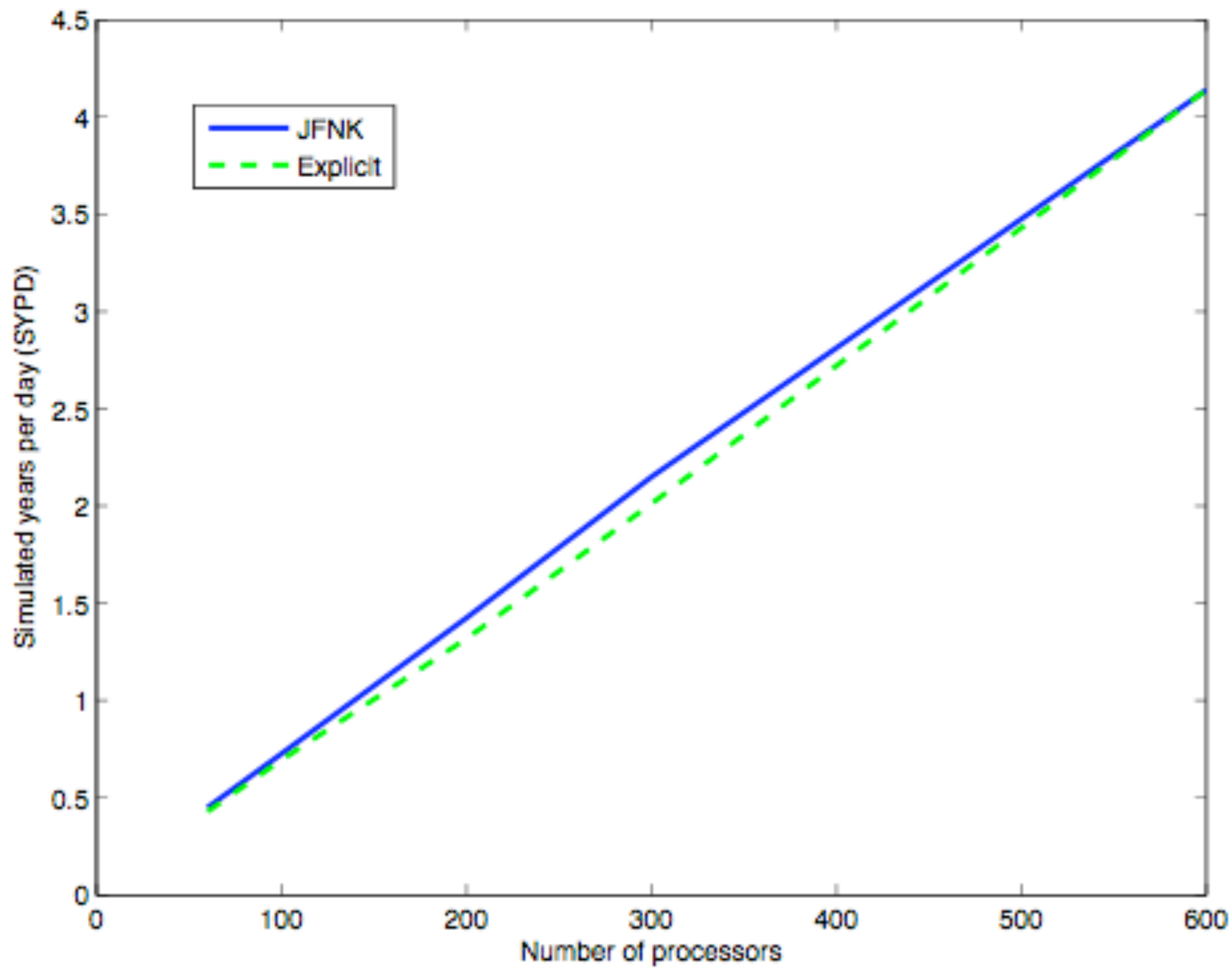
Test case 1: cosine bell initial condition



Strong scaling

- 6 x 10 x 10 elements
- 16 x 16 points per element
- 26 vertical levels
- Fixed problem size, increase processes
- Explicit versus <u>unpreconditioned</u> JFNK
  - 30 s time step for explicit
  - 720 s time step for JFNK
  - Similar L_2 error

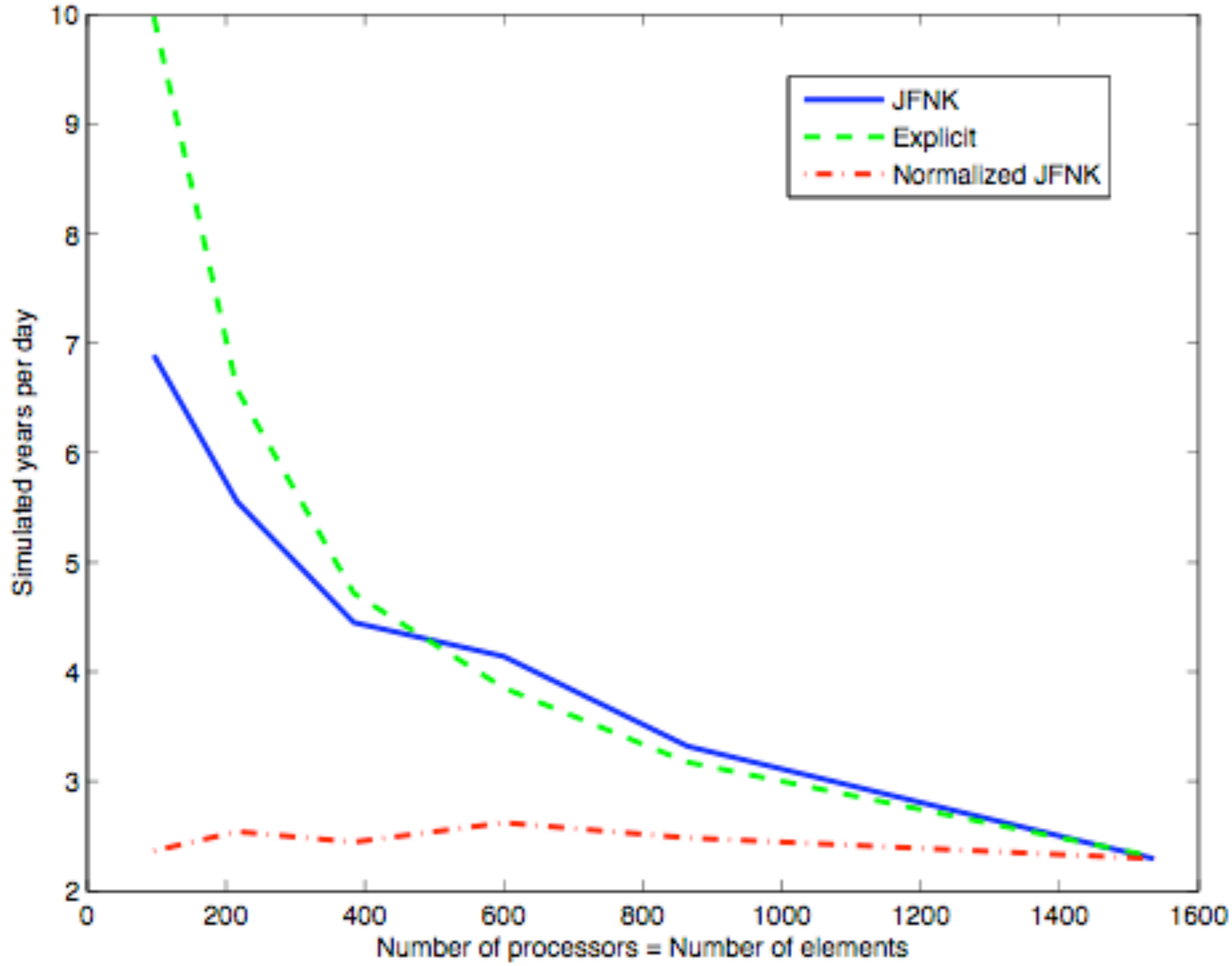
Strong scaling on Jaguar



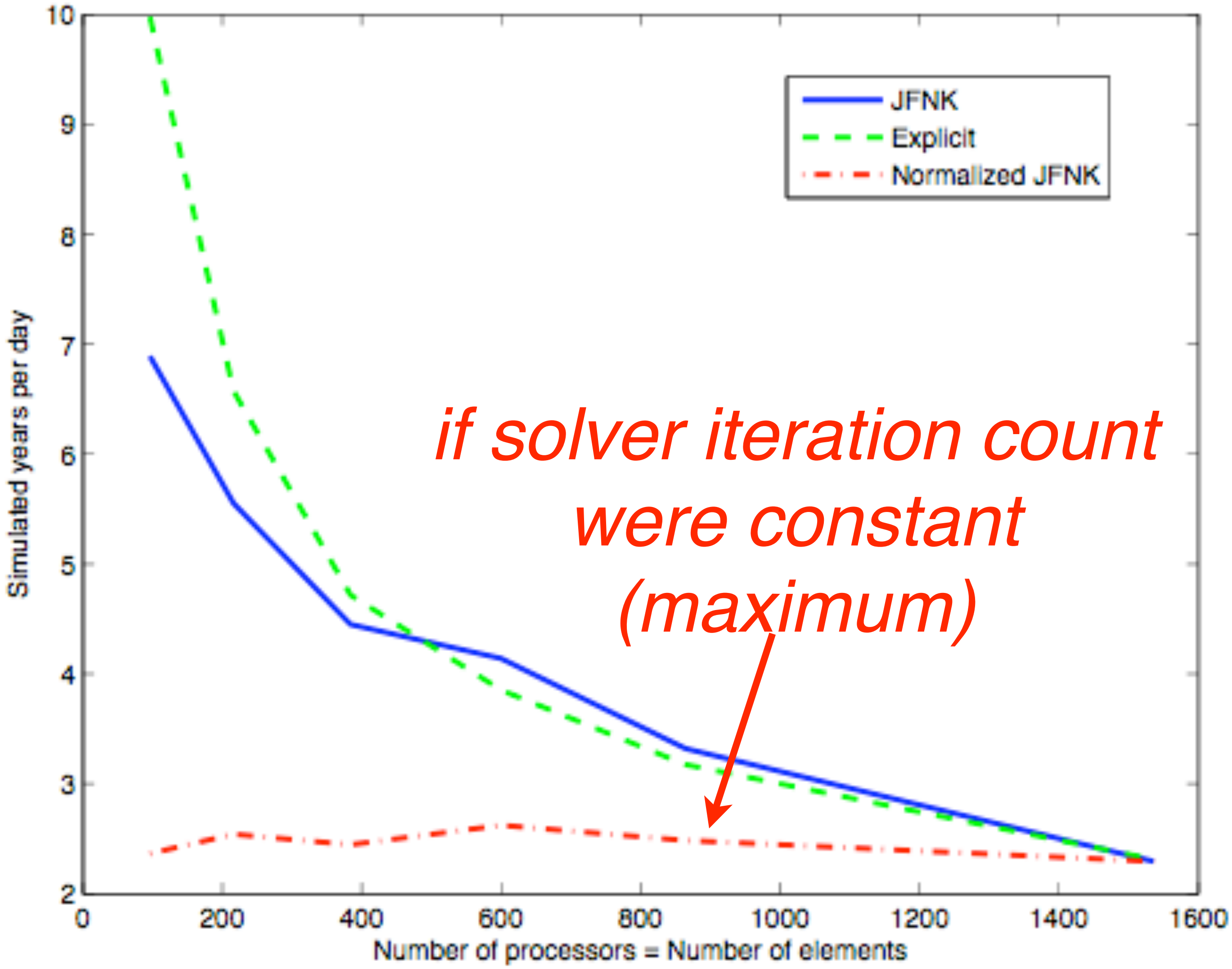
Weak scaling

- 6 x (4 x 4 to 10 x 10) elements
- 16 x 16 points per element
- 26 vertical levels
- Constant number of elements per process
- Increase processes
- Explicit versus <u>unpreconditioned</u> JFNK
  - Shrinking time step for explicit
  - Constant 720 s time step for JFNK
  - But increasing iterations per solve

Weak scaling on Jaguar

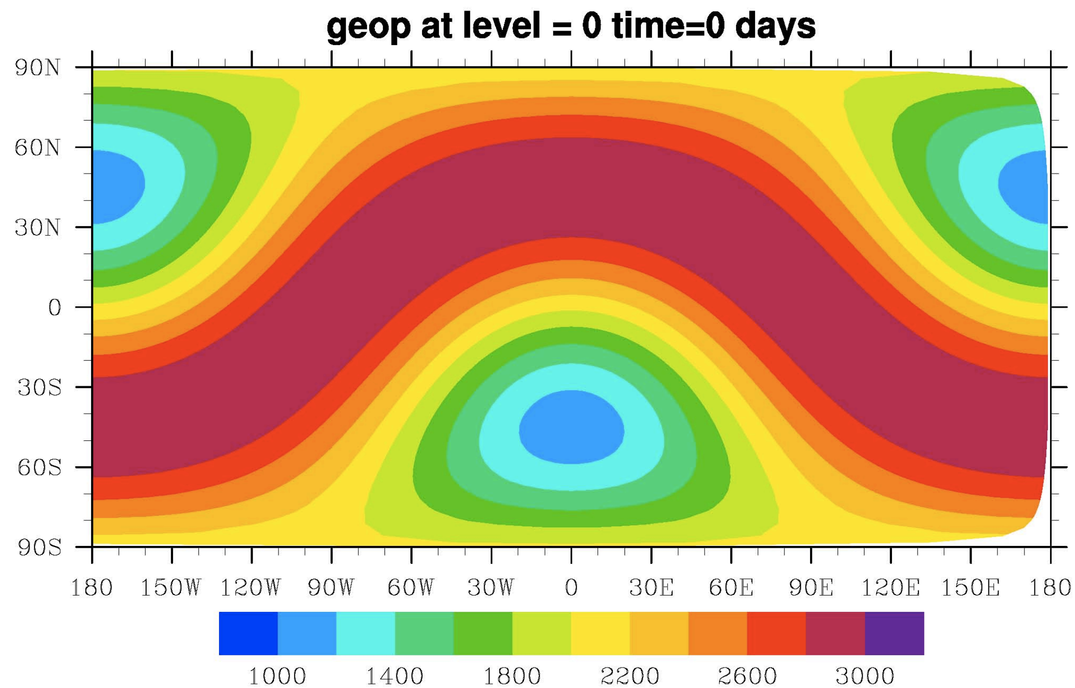


Weak scaling

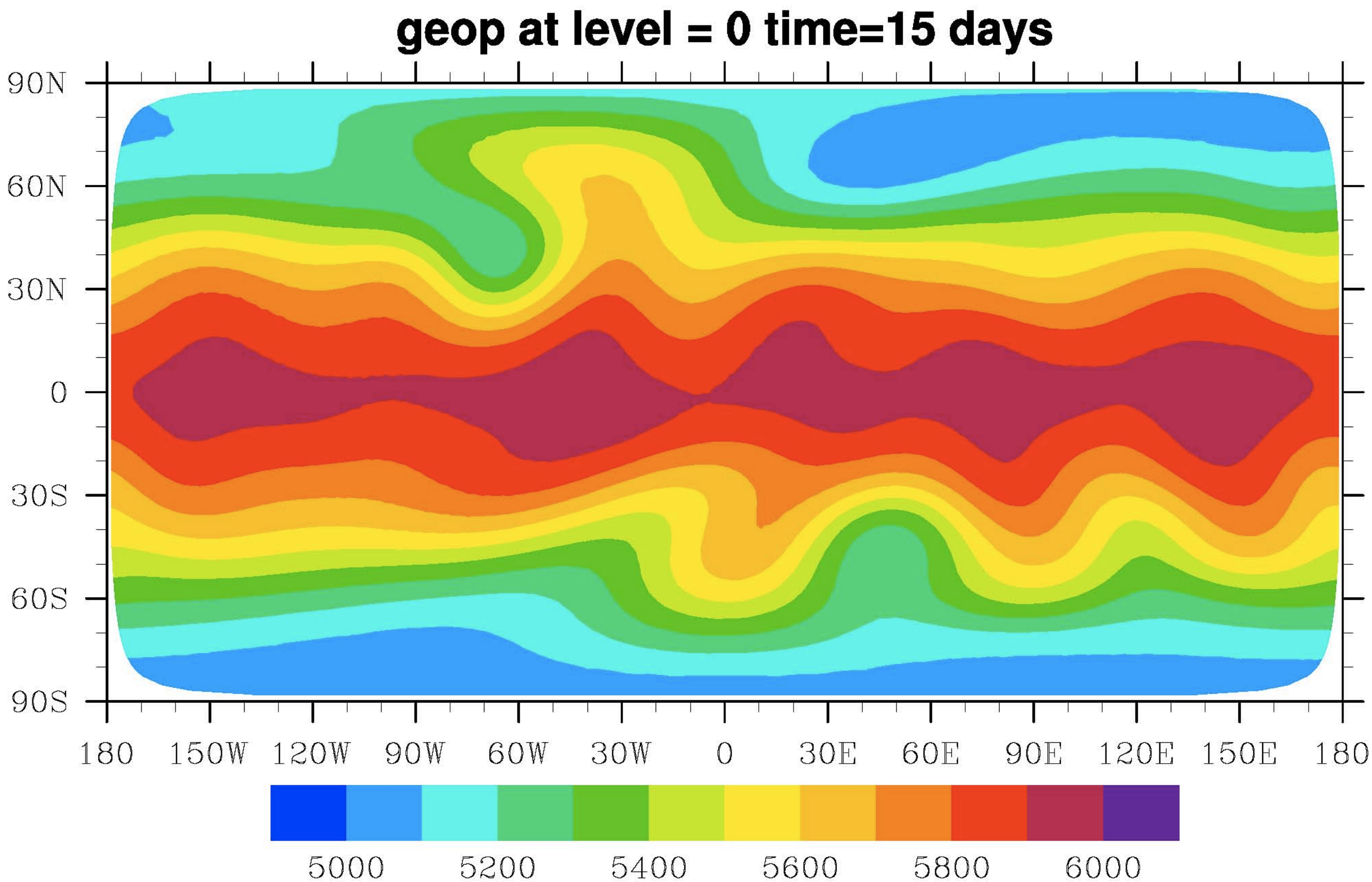


Test case 2: steady state

- 12 simulated days
- Explicit
  - 4-minute time step
  - 28s runtime
- Implicit
  - 12-day time step
  - 3.6s runtime



Test case 5: Flow over a mountain

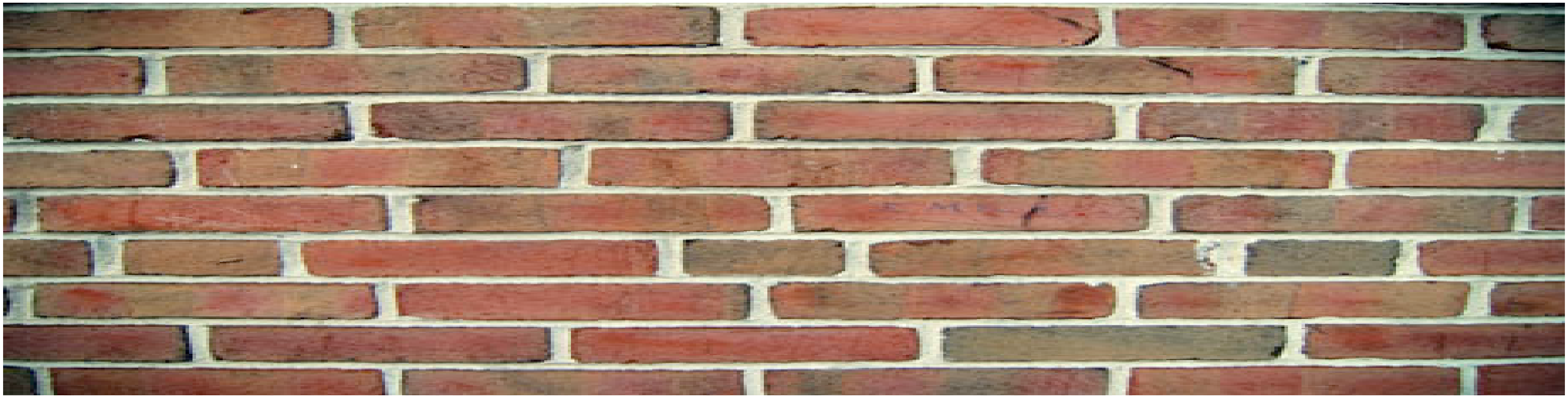


Potential Preconditioners

- Semi-implicit solver
- Overlapping Schwarz
- Multigrid with overlapping-Schwarz smoother
- Lott and Elman (U of MD) spectral-element preconditioner

Overcoming the time barrier

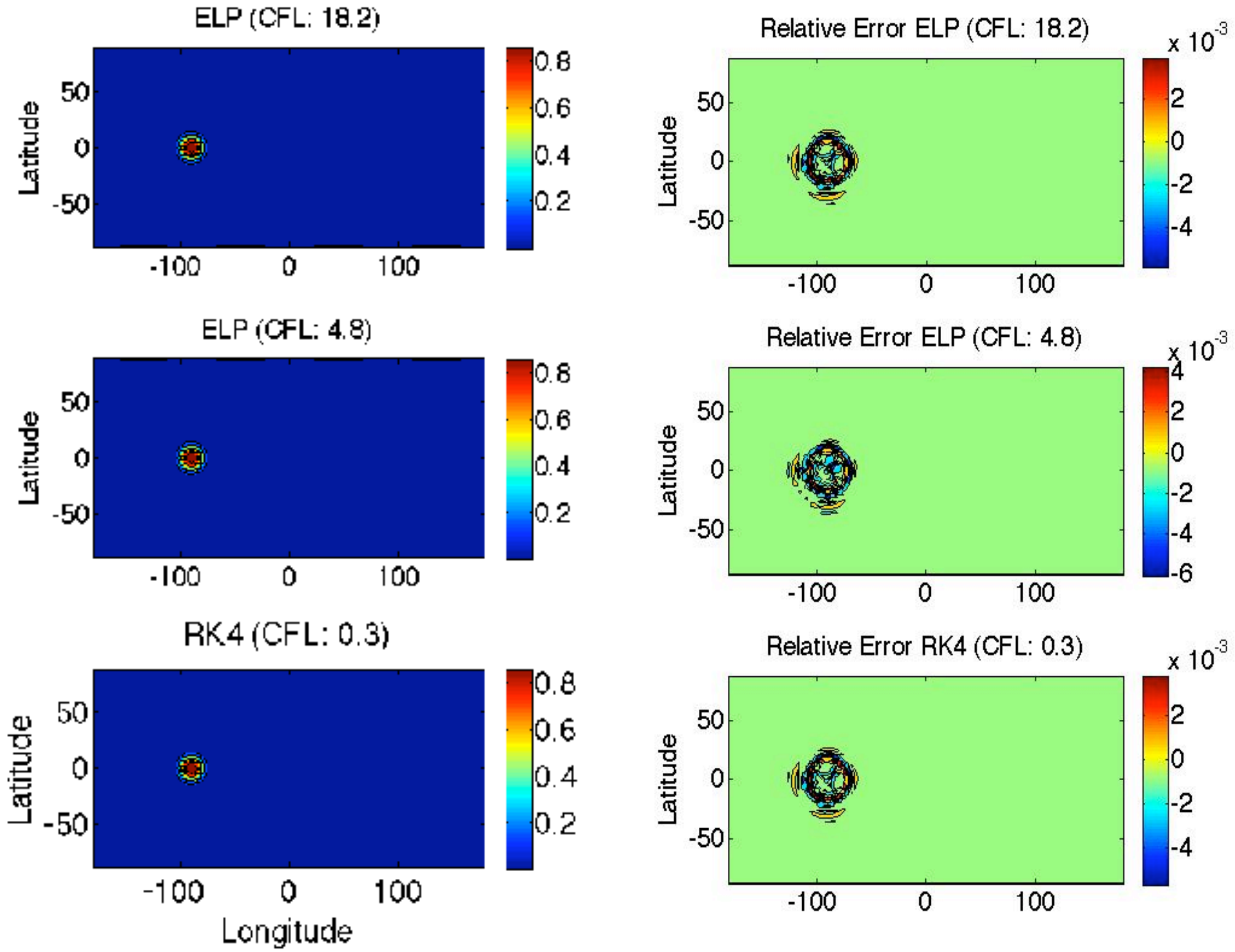
- Fully implicit time integration
- Multiwavelet discontinuous Galerkin
- Parareal



Multiwavelet discontinuous Galerkin
(Rick Archibald)

- Multiwavelet basis
  - Adaptive
  - Sparse
- Discontinuous Galerkin on cubed sphere
- Exact Linear Part (ELP) time integration
  - Allows large time steps at high accuracy
  - Multiwavelets maintain sparsity

Test case 1


ELP (CFL: 18.2)
Relative Error ELP (CFL: 18.2)
ELP (CFL: 4.8)
Relative Error ELP (CFL: 4.8)
RK4 (CFL: 0.3)
Relative Error RK4 (CFL: 0.3)
Latitude
Longitude
x 10^-3

Test case 1

Table 1. Convergence rates for Example 1 using RK4 and ELP time stepping for the multiwavelet DG method with order $k = 3$ and drop tolerance $\epsilon = 10^{-4}$ for the ELP with CFL= 4.8 and $\epsilon = 10^{-5}$ otherwise. The number of non-zero elements for each operator is give by N_z.

	RK4 (CFL = 0.3)			ELP (CFL = 4.8)			ELP (CFL = 18.2)		
N	L_2 error	Order	N_z	L_2 error	Order	N_z	L_2 error	Order	N_z
cosine bell									
4	1.98e-1	-	5.7e5	1.98e-1	-	5.9e5	1.96e-1	-	1.5e6
8	4.04e-2	2.30	2.4e6	4.18e-2	2.25	2.5e6	4.11e-2	2.26	8.2e6
16	7.53e-3	2.42	9.9e6	7.61e-3	2.46	1.0e7	7.71e-3	2.14	3.4e7
Gaussian hill									
4	2.0e-2	-	5.7e5	2.01e-2	-	5.9e5	2.02e-2	-	1.5e6
8	3.04e-3	2.72	2.4e6	3.06e-3	2.72	2.5e6	3.08e-3	2.72	8.2e6
16	3.6e-4	3.09	9.9e6	3.62e-4	3.08	1.0e7	3.63e-4	3.08	3.4e7

Test case 1

Table 1. Convergence rates for Example 1 using RK4 and ELP time stepping for the multiwavelet DG method with order $k = 3$ and drop tolerance $\epsilon = 10^{-4}$ for the ELP with CFL= 4.8 and $\epsilon = 10^{-5}$ otherwise. The number of non-zero elements for each operator is give by N_z.

Up to 60x time step

	RK4 (CFL = 0.3)			ELP (CFL = 4.8)			ELP (CFL = 18.2)		
N	L_2 error	Order	N_z	L_2 error	Order	N_z	L_2 error	Order	N_z
cosine bell									
4	1.98e-1	-	5.7e5	1.98e-1	-	5.9e5	1.96e-1	-	1.5e6
8	4.04e-2	2.30	2.4e6	4.18e-2	2.25	2.5e6	4.11e-2	2.26	8.2e6
16	7.53e-3	2.42	9.9e6	7.61e-3	2.46	1.0e7	7.71e-3	2.14	3.4e7
Gaussian hill									
4	2.0e-2	-	5.7e5	2.01e-2	-	5.9e5	2.02e-2	-	1.5e6
8	3.04e-3	2.72	2.4e6	3.06e-3	2.72	2.5e6	3.08e-3	2.72	8.2e6
16	3.6e-4	3.09	9.9e6	3.62e-4	3.08	1.0e7	3.63e-4	3.08	3.4e7

Test case 1

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N	L_2 error	Order	N_z	L_2 error	Order	N_z	L_2 error	Order	N_z
cosine bell									
4	1.98e-1	-	5.7e5	1.98e-1	-	5.9e5	1.96e-1	-	1.5e6
8	4.04e-2	2.30	2.4e6	4.18e-2	2.25	2.5e6	4.11e-2	2.26	8.2e6
16	7.53e-3	2.42	9.9e6	7.61e-3	2.46	1.0e7	7.71e-3	2.14	3.4e7
Gaussian hill									
4	2.0e-2	-	5.7e5	2.01e-2	-	5.9e5	2.02e-2	-	1.5e6
8	3.04e-3	2.72	2.4e6	3.06e-3	2.72	2.5e6	3.08e-3	2.72	8.2e6
16	3.6e-4	3.09	9.9e6	3.62e-4	3.08	1.0e7	3.63e-4	3.08	3.4e7

Identical L_2 error

Test case 1

Table 1. Convergence rates for Example 1 using RK4 and ELP time stepping for the multiwavelet DG method with order $k = 3$ and drop tolerance $\epsilon = 10^{-4}$ for the ELP with CFL$= 4.8$ and $\epsilon = 10^{-5}$ otherwise. The number of non-zero elements for each operator is give by N_z.

	RK4 (CFL = 0.3)			ELP (CFL = 4.8)			ELP (CFL = 18.2)		
N	L_2 error	Order	N_z	L_2 error	Order	N_z	L_2 error	Order	N_z
cosine bell									
4	1.98e-1	-	5.7e5	1.98e-1	-	5.9e5	1.96e-1	-	1.5e6
8	4.04e-2	2.30	2.4e6	4.18e-2	2.25	2.5e6	4.11e-2	2.26	8.2e6
16	7.53e-3	2.42	9.9e6	7.61e-3	2.46	1.0e7	7.71e-3	2.14	3.4e7
Gaussian hill									
4	2.0e-2	-	5.7e5	2.01e-2	-	5.9e5	2.02e-2	-	1.5e6
8	3.04e-3	2.72	2.4e6	3.06e-3	2.72	2.5e6	3.08e-3	2.72	8.2e6
16	3.6e-4	3.09	9.9e6	3.62e-4	3.08	1.0e7	3.63e-4	3.08	3.4e7

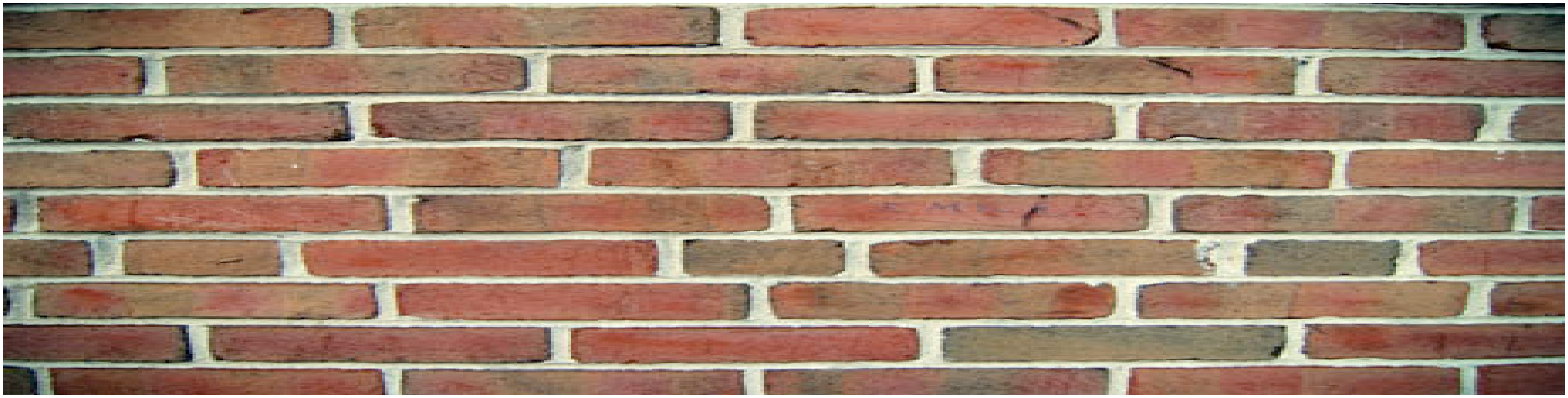
3x change in sparsity

Multiwavelet DG

- Early results for nonlinear test cases are promising

Overcoming the time barrier

- Fully implicit time integration
- Multiwavelet discontinuous Galerkin
- Parareal



Parareal

- Algorithm published in 2001 by Jacques-Louis Lions, Yvon Maday, and Gabriel Turinici
- Variants successful for range of applications
  - Navier-Stokes
  - Structural dynamics
  - Reservoir simulation

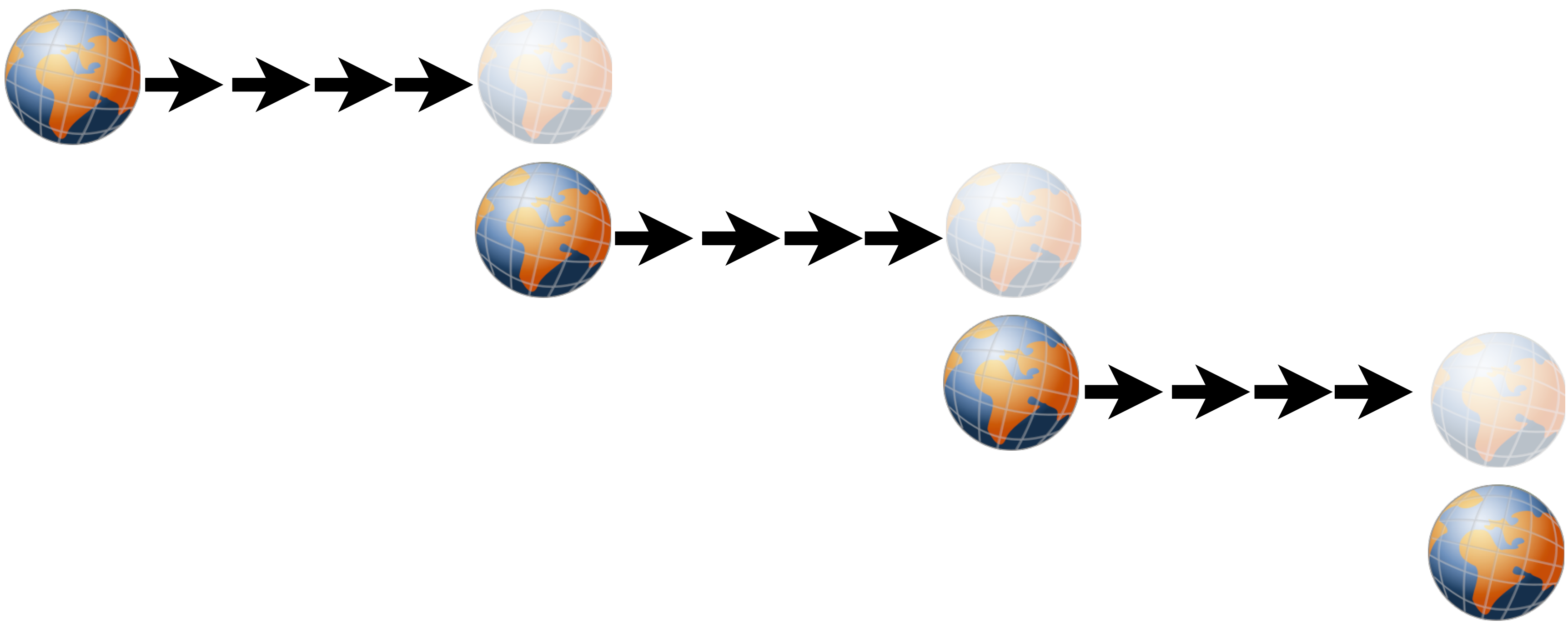
Lions

Maday

Parareal

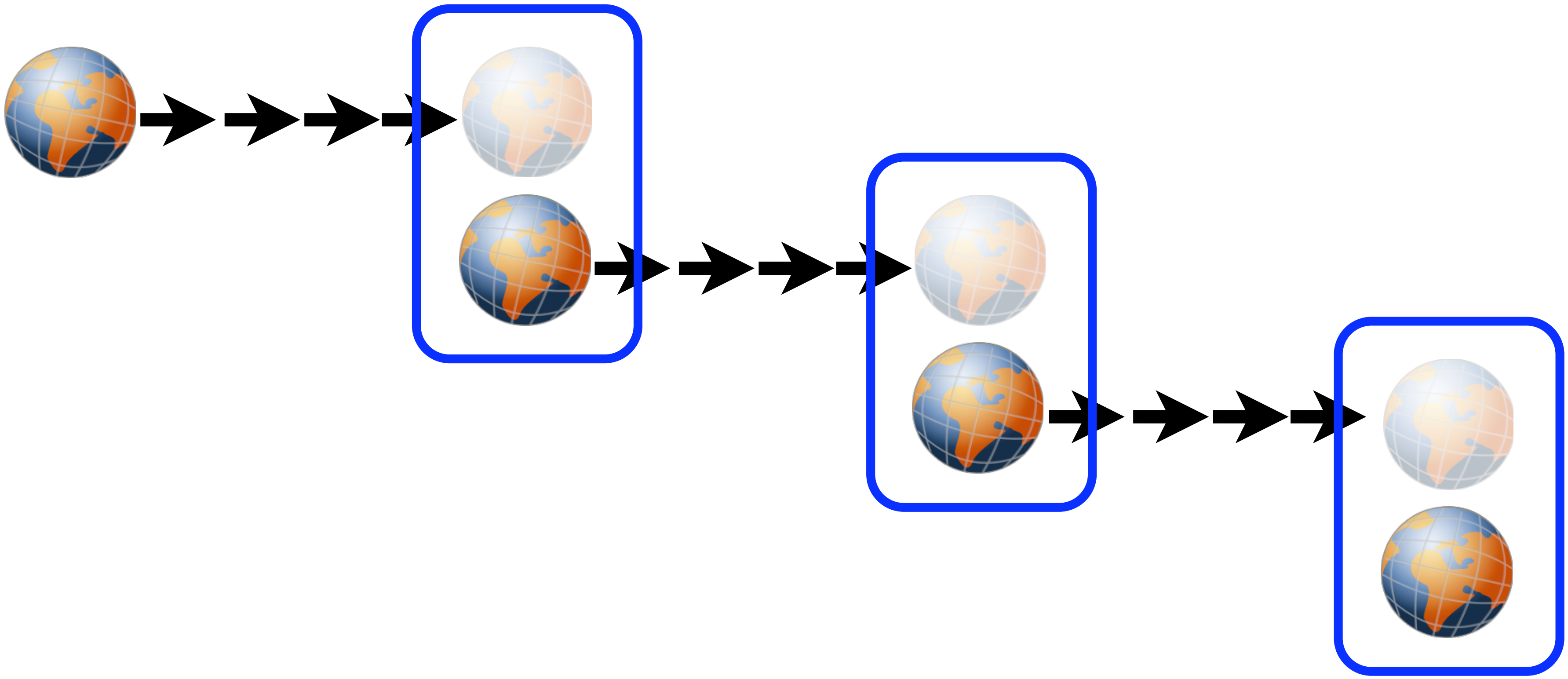
Start with serial coarse time steps

Parareal



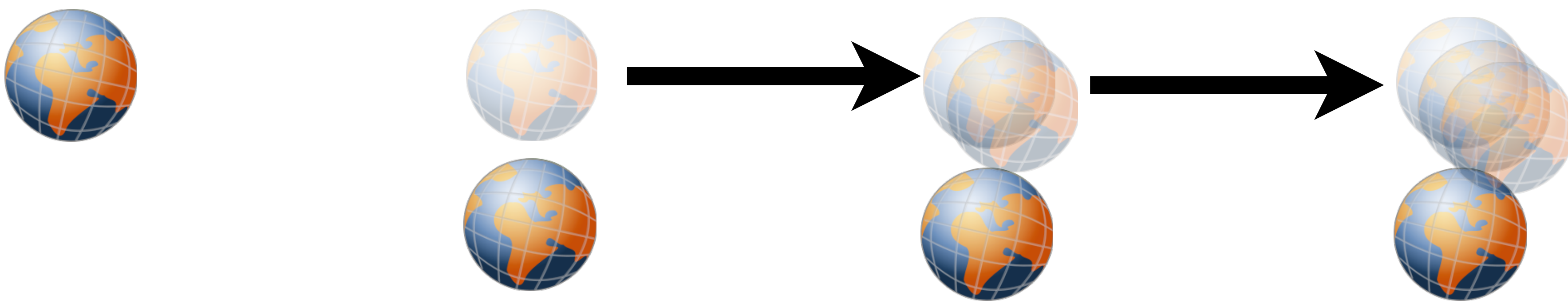
Starting from coarse points,
do fine time steps in parallel

Parareal



Get fine-scale corrections to coarse states

Parareal



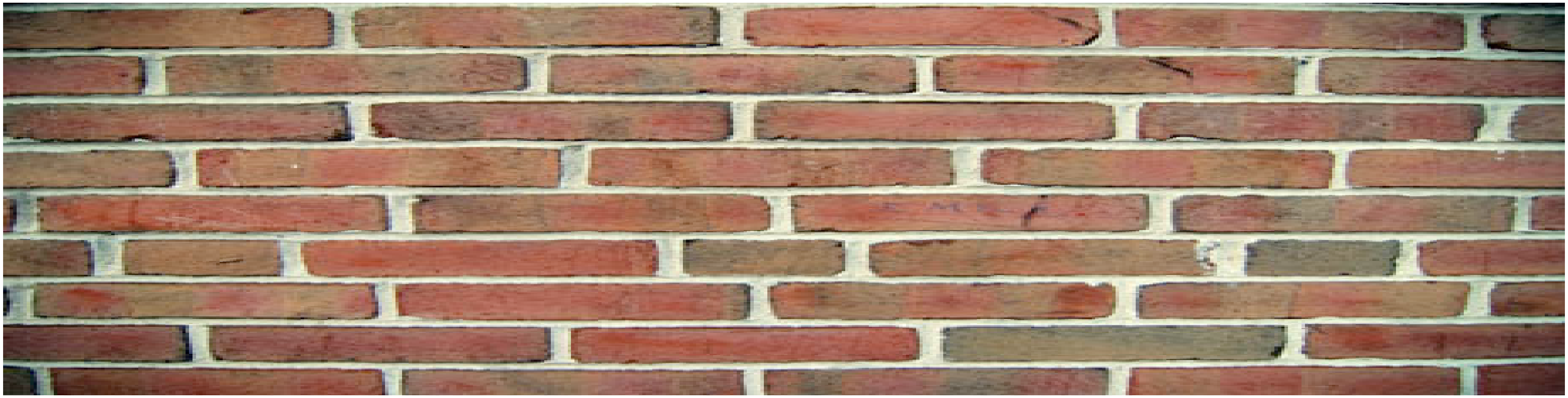
Propagate <u>accumulated</u> corrections
<u>serially</u> with coarse time step

Parareal

- Iterate until corrections are negligible
- Published results by others: 2-3 iterations
- We have success with 1D Burgers
  - Relevant?
- Stable integration of advection-dominated problems will be a challenge

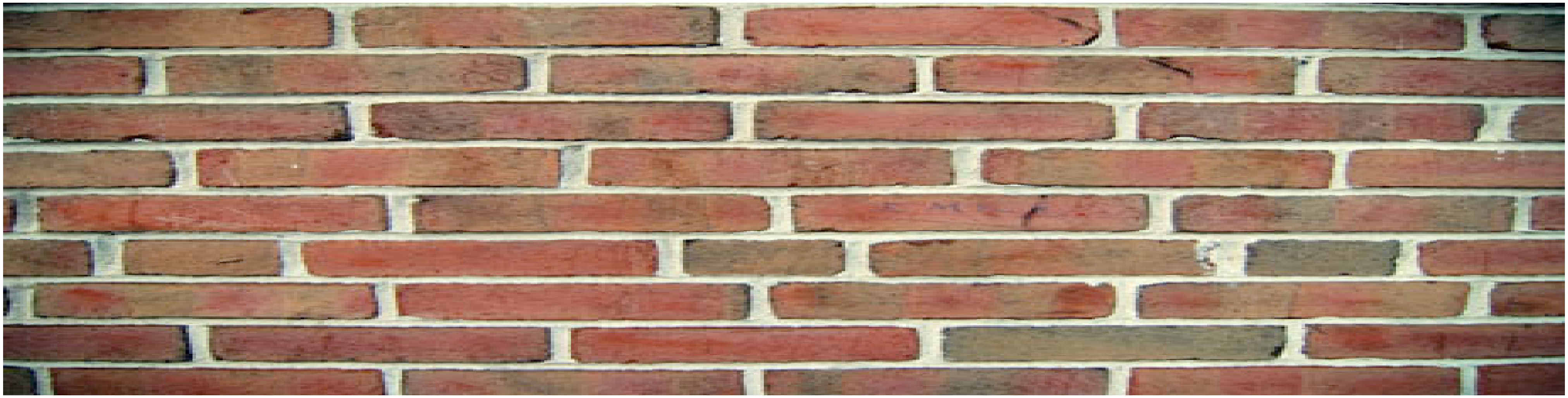
Overcoming the time barrier

- Fully implicit time integration
- Multiwavelet discontinuous Galerkin
- Parareal



Overcoming the time barrier

- Fully implicit time integration
  - Preconditioners
- Multiwavelet discontinuous Galerkin
  - Nonlinear problems
  - Parallel implementation
- Parareal
  - Stability for advection



MS82
Scalable Dynamical Cores for Climate and Weather Modeling

Title not available at time of publication

Overcoming the Time Barrier

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Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U. S. Department of Energy under Contract No. DE-AC05-00OR22725.

This research used resources of the National Center for Computational Sciences at Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

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